

Match level :

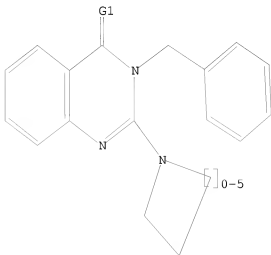
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
 21:Atom 22:Atom 23:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:44:50 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 176 TO ITERATE

100.0% PROCESSED 176 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 2725 TO 4315

PROJECTED ANSWERS: 6 TO 266

L2 6 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 14:44:57 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3468 TO ITERATE

100.0% PROCESSED 3468 ITERATIONS
SEARCH TIME: 00.00.01

127 ANSWERS

L3 127 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

185.88

186.10

FILE 'CAPLUS' ENTERED AT 14:45:02 ON 25 MAR 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 25 Mar 2009 VOL 150 ISS 13

FILE LAST UPDATED: 24 Mar 2009 (20090324/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 4 L3

=> d ibib abs hitstr tot

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS ON STM

ACCESSION NUMBER: 2009:779820 CAPLUS

149118493

DOCUMENT NUMBER: Discovery of alopiptin: A potent, selective, bioavailable, and efficacious inhibitor of dipeptidyl peptidase IV. (Excerpt to document cited in CA147-045193)

AUTHOR(S): Peng, Jun; Chang, Shiyuan; Wallace, Michael B.; Stafford, Jeffrey A.; Kaidor, Stephen W.; Kassel, Daniel R.; Hays, Mary Shi, Lihong; Shen, Robert

J. J.

Asakawa, Tomohiko; Takemachi, Ryoji; Xu, Hongda; Webb, David B.; Swelling, Stephen L. Takeda San Diego, Inc., San Diego, CA, 92121, USA. Journal of Medicinal Chemistry 12009, 52(14), 4357. CODES: JMCMA5, ISSN: 0022-2625

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB On page 2297, Figure 1 is incorrect; the correct version of the figure is given. On page 2298, Figure 4 is incorrect; the correct version of the figure is given.

IT 763157-63-3P 763157-71-3P 940907-93-7P

940907-94-8P 940907-85-9P 940907-97-1P

940907-99-3P 940908-00-3P 940908-01-0P

940908-02-1P 940908-03-2P 940908-05-4P

940908-07-6P

E2: PAC (Pharmacological activity); PKT (Pharmacokinetics); STM

(Synthetic preparation); THO (Therapeutic use); BIO: (Biological study); PREP

(Preparation); PREP (Preparation)

(Discovery of alopiptin, a potent, selective, bioavailable, and

efficacious inhibitor of dipeptidyl peptidase IV (Erratum))

J2: 763157-63-3 CAPLUS

C2: Benzonitrile,

2-[[2-[(3R)-3-amino-1-piperidinyl]-7-fluoro-6-methoxy-6-oxo-

3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1

C2: 763157-70-2

C2: 940907-93-7

C2: 940907-94-8

C2: 940907-97-1

C2: 940908-00-3

C2: 940908-01-0

C2: 940908-02-1

C2: 940908-03-2

C2: 940908-05-4

C2: 940908-07-6

C2: 940908-08-7

C2: 940908-09-8

C2: 940908-10-9

C2: 940908-11-0

C2: 940908-12-1

C2: 940908-13-2

C2: 940908-14-3

C2: 940908-15-4

C2: 940908-16-5

C2: 940908-17-6

C2: 940908-18-7

C2: 940908-19-8

C2: 940908-20-9

C2: 940908-21-0

C2: 940908-22-1

C2: 940908-23-2

C2: 940908-24-3

C2: 940908-25-4

C2: 940908-26-5

C2: 940908-27-6

C2: 940908-28-7

C2: 940908-29-8

C2: 940908-30-9

C2: 940908-31-0

C2: 940908-32-1

C2: 940908-33-2

C2: 940908-34-3

C2: 940908-35-4

C2: 940908-36-5

C2: 940908-37-6

C2: 940908-38-7

C2: 940908-39-8

C2: 940908-40-9

C2: 940908-41-0

C2: 940908-42-1

C2: 940908-43-2

C2: 940908-44-3

C2: 940908-45-4

C2: 940908-46-5

C2: 940908-47-6

C2: 940908-48-7

C2: 940908-49-8

C2: 940908-50-9

C2: 940908-51-0

C2: 940908-52-1

C2: 940908-53-2

C2: 940908-54-3

C2: 940908-55-4

C2: 940908-56-5

C2: 940908-57-6

C2: 940908-58-7

C2: 940908-59-8

C2: 940908-60-9

C2: 940908-61-0

C2: 940908-62-1

C2: 940908-63-2

C2: 940908-64-3

C2: 940908-65-4

C2: 940908-66-5

C2: 940908-67-6

C2: 940908-68-7

C2: 940908-69-8

C2: 940908-70-9

C2: 940908-71-0

C2: 940908-72-1

C2: 940908-73-2

C2: 940908-74-3

C2: 940908-75-4

C2: 940908-76-5

C2: 940908-77-6

C2: 940908-78-7

C2: 940908-79-8

C2: 940908-80-9

C2: 940908-81-0

C2: 940908-82-1

C2: 940908-83-2

C2: 940908-84-3

C2: 940908-85-4

C2: 940908-86-5

C2: 940908-87-6

C2: 940908-88-7

C2: 940908-89-8

C2: 940908-90-9

C2: 940908-91-0

C2: 940908-92-1

C2: 940908-93-2

C2: 940908-94-3

C2: 940908-95-4

C2: 940908-96-5

C2: 940908-97-6

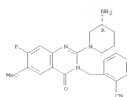
C2: 940908-98-7

C2: 940908-99-8

C2: 940908-100-9

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS ON STM

(Continued)



CH 2

C2: 76-05-1

C2: 940907-93-7



R2: 763157-71-3 CAPLUS

C2: Benzonitrile, 2-[[2-[(3R)-3-amino-1-piperidinyl]-5-fluoro-4-oxo-3(4H)-

quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1

C2: 763157-70-2

C2: 940907-93-7

Absolute stereochemistry.

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS ON STM (Continued)

ACCESSION NUMBER: 2009:779820 CAPLUS

149118493

DOCUMENT NUMBER: Discovery of alopiptin: A potent, selective, bioavailable, and efficacious inhibitor of dipeptidyl peptidase IV. (Excerpt to document cited in CA147-045193)

AUTHOR(S): Peng, Jun; Chang, Shiyuan; Wallace, Michael B.; Stafford, Jeffrey A.; Kaidor, Stephen W.; Kassel, Daniel R.; Hays, Mary Shi, Lihong; Shen, Robert

J. J.

Asakawa, Tomohiko; Takemachi, Ryoji; Xu, Hongda; Webb, David B.; Swelling, Stephen L. Takeda San Diego, Inc., San Diego, CA, 92121, USA. Journal of Medicinal Chemistry 12009, 52(14), 4357. CODES: JMCMA5, ISSN: 0022-2625

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB On page 2297, Figure 1 is incorrect; the correct version of the figure is given. On page 2298, Figure 4 is incorrect; the correct version of the figure is given.

IT 763157-63-3P 763157-71-3P 940907-93-7P

940907-94-8P 940907-85-9P 940907-97-1P

940907-99-3P 940908-00-3P 940908-01-0P

940908-02-1P 940908-03-2P 940908-05-4P

940908-07-6P

E2: PAC (Pharmacological activity); PKT (Pharmacokinetics); STM

(Synthetic preparation); THO (Therapeutic use); BIO: (Biological study); PREP

(Preparation); PREP (Preparation)

(Discovery of alopiptin, a potent, selective, bioavailable, and

efficacious inhibitor of dipeptidyl peptidase IV (Erratum))

J2: 763157-63-3 CAPLUS

C2: Benzonitrile,

2-[[2-[(3R)-3-amino-1-piperidinyl]-4-oxo-3(4H)-

quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1

C2: 763157-70-2

C2: 940907-93-7

C2: 940907-94-8

C2: 940907-97-1

C2: 940908-00-3

C2: 940908-01-0

C2: 940908-02-1

C2: 940908-03-2

C2: 940908-05-4

C2: 940908-07-6

C2: 940908-08-7

C2: 940908-09-8

C2: 940908-10-9

C2: 940908-11-0

C2: 940908-12-1

C2: 940908-13-2

C2: 940908-14-3

C2: 940908-15-4

C2: 940908-16-5

C2: 940908-17-6

C2: 940908-18-7

C2: 940908-19-8

C2: 940908-20-9

C2: 940908-21-0

C2: 940908-22-1

C2: 940908-23-2

C2: 940908-24-3

C2: 940908-25-4

C2: 940908-26-5

C2: 940908-27-6

C2: 940908-28-7

C2: 940908-29-8

C2: 940908-30-9

C2: 940908-31-0

C2: 940908-32-1

C2: 940908-33-2

C2: 940908-34-3

C2: 940908-35-4

C2: 940908-36-5

C2: 940908-37-6

C2: 940908-38-7

C2: 940908-39-8

C2: 940908-40-9

C2: 940908-41-0

C2: 940908-42-1

C2: 940908-43-2

C2: 940908-44-3

C2: 940908-45-4

C2: 940908-46-5

C2: 940908-47-6

C2: 940908-48-7

C2: 940908-49-8

C2: 940908-50-9

C2: 940908-51-0

C2: 940908-52-1

C2: 940908-53-2

C2: 940908-54-3

C2: 940908-55-4

C2: 940908-56-5

C2: 940908-57-6

C2: 940908-58-7

C2: 940908-59-8

C2: 940908-60-9

C2: 940908-61-0

C2: 940908-62-1

C2: 940908-63-2

C2: 940908-64-3

C2: 940908-65-4

C2: 940908-66-5

C2: 940908-67-6

C2: 940908-68-7

C2: 940908-69-8

C2: 940908-70-9

C2: 940908-71-0

C2: 940908-72-1

C2: 940908-73-2

C2: 940908-74-3

C2: 940908-75-4

C2: 940908-76-5

C2: 940908-77-6

C2: 940908-78-7

C2: 940908-79-8

C2: 940908-80-9

C2: 940908-81-0

C2: 940908-82-1

C2: 940908-83-2

C2: 940908-84-3

C2: 940908-85-4

C2: 940908-86-5

C2: 940908-87-6

C2: 940908-88-7

C2: 940908-89-8

C2: 940908-90-9

C2: 940908-

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

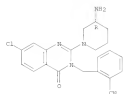
CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



BN 940907-97-1 CAPLUS
 CN Benzonitrile, 2-[[12-[(1R)-3-amino-1-piperidinyl]-7-chloro-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1
 CHN 940907-96-0
 CNF C21 H20 Cl N5 O

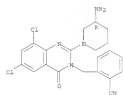
Absolute stereochemistry.



CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



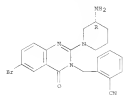
CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



BN 940908-01-0 CAPLUS
 CN Benzonitrile, 2-[[12-[(1R)-3-amino-1-piperidinyl]-6-bromo-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1
 CHN 761517-99-3
 CNF C21 H20 Br N5 O

Absolute stereochemistry.



CH 2

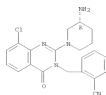
Habe

14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

BN 940907-99-3 CAPLUS
 CN Benzonitrile, 2-[[12-[(1R)-3-amino-1-piperidinyl]-8-chloro-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1
 CHN 940907-98-2
 CNF C21 H20 Cl N5 O

Absolute stereochemistry.



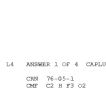
CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



BN 940908-02-9 CAPLUS
 CN Benzonitrile, 2-[[12-[(1R)-3-amino-1-piperidinyl]-6,8-dichloro-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1
 CHN 761517-99-9
 CNF C21 H19 Cl2 N5 O

Absolute stereochemistry.



14 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

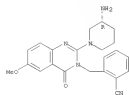
CHN 76-05-1
 CNF C2 H F3 O2



BN 940908-02-1 CAPLUS
 CN Benzonitrile, 2-[[12-[(1R)-3-amino-1-piperidinyl]-6-methoxy-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1
 CHN 761517-99-9
 CNF C22 H23 N5 O2

Absolute stereochemistry.



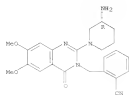
CH 2
 CHN 76-05-1
 CNF C2 H F3 O2



BN 940908-02-2 CAPLUS
 CN Benzonitrile, 2-[[12-[(1R)-3-amino-1-piperidinyl]-4,7-dimethoxy-4-oxo-3(4H)-quinazolinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 4 CAPLOS COPYRIGHT 2009 ACS ON STN (Continued)

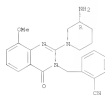


IN 940908-04-3 CAPLOS
CN Benzonitrile, 2-[(2-[(1R)-3-amino-1-piperidinyl]-8-methoxy-4-oxo-3(4H)-quinazolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1

CHI 940908-04-3
CHI C22 R23 R5 O2

Absolute stereochemistry.



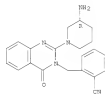
CN 2

CHI 76-05-1
CHI C2 R F3 O2

L4 ANSWER 1 OF 4 CAPLOS COPYRIGHT 2009 ACS ON STN (Continued)

CN Benzonitrile, 2-[(2-[(1R)-3-amino-1-piperidinyl]-4-oxo-3(4H)-quinazolinyl)methyl]-, (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 1 OF 4 CAPLOS COPYRIGHT 2009 ACS ON STN (Continued)



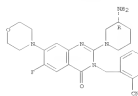
IN 940908-07-5 CAPLOS

CN Benzonitrile, 2-[(2-[(1R)-3-amino-1-piperidinyl]-4-fluoro-7-[4-morpholinyl]-6-oxo-3(4H)-quinazolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1

CHI 76157-95-1
CHI C25 R27 F R6 O2

Absolute stereochemistry.



CN 2

CHI 76-05-1
CHI C2 R F3 O2



IT 940907-93-TDP, complex with dipeptidyl peptidase IV

RI: PRP (Preparation); SRH (Synthetic preparation); PREP (Preparation) (discovery of alogliptin, a potent, selective, bioavailable, and efficacious inhibitor of dipeptidyl peptidase IV (Erstatin))

IN 940907-93-7 CAPLOS

L4 ANSWER 2 OF 4 CAPLOS COPYRIGHT 2009 ACS ON STN

ACCESSION NUMBER: 2007167845 CAPLOS
DOI: 10.1021/acs.chem.1c00001

TITLE: Discovery of Alogliptin: A Potent, Selective, Bioavailable, and Efficacious Inhibitor of Dipeptidyl Peptidase IV

AUTHOR(S): Feng, Juny; Zhang, Zhiyuan; Wallace, Michael S.; Stafford, Jeffrey A.; Walder, Stephen W.; Kessel, Daniel S.; Nave, Marc; Shi, Liang; Skene, Robert J.

J.: Aikawa, Tomoko; Takouchi, Keiji; Xu, Hong; Webb, David S.; Oellrich, Stephen L., II
Takeda San Diego, Inc., San Diego, CA, 92121, USA
JOURNAL OF MEDICAL CHEMISTRY (2007), 50(10), 2287-2300

CODEN: JMCMDJ; ISSN: 0022-2625

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CHEMREACT 147:45103

AB Alogliptin is a potent, selective inhibitor of the serine protease dipeptidyl peptidase IV (DPP-4). Herein, the authors describe the structure-based design and optimization of alogliptin and related quinazolinone-based DPP-4 inhibitors. Following an oral dose, these noncovalent inhibitors provide sustained reduction of plasma DPP-4 activity and a lowering of blood glucose in animal models of diabetes. Alogliptin is currently undergoing phase III trials in patients with type 2 diabetes.

IT 76157-65-5P 76157-71-3P 940907-93-7P

940907-94-8P 940907-95-9P 940907-97-1P

940907-98-2P 940908-00-3P 940908-01-0P

940908-02-1P 940908-03-2P 940908-05-4P

940908-07-6P

RI: PNC (Pharmacokinetic activity); PRP (Pharmacokinetics); SRH (Preparation); SRH (Therapeutic use); RIOL (Biological study); PREP (Preparation); USR (Use)

(discovery of alogliptin, a potent, selective, bioavailable, and efficacious inhibitor of dipeptidyl peptidase IV)

IN 76157-65-5 CAPLOS

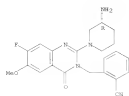
CN Benzonitrile, 2-[(2-[(1R)-3-amino-1-piperidinyl]-7-fluoro-6-methoxy-3(4H)-quinazolinyl)methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CN 1

CHI 76157-64-4
CHI C22 R22 F R5 O2

Absolute stereochemistry.

L4 ANSWER 2 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)



CM 2
 CHN 76-05-1
 CHF C2 H F3 O2

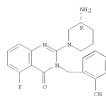


RI 769157-71-3 CAPLOS
 RI Benzonitrile, 2-[[12-[(3R)-3-amino-1-piperidinyl]-5-fluoro-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1
 CHN 769157-70-2
 CHF C21 H20 F N5 O

Absolute stereochemistry.

L4 ANSWER 2 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)

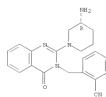


CM 2
 CHN 76-05-1
 CHF C2 H F3 O2



RI 940907-93-7 CAPLOS
 RI Benzonitrile, 2-[[12-[(3R)-3-amino-1-piperidinyl]-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

Absolute stereochemistry.

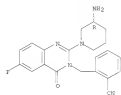


RI 940907-94-8 CAPLOS
 RI Benzonitrile, 2-[[12-[(3R)-3-amino-1-piperidinyl]-5-fluoro-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

L4 ANSWER 2 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)

CM 1
 CHN 769158-14-7
 CHF C21 H20 F N5 O

Absolute stereochemistry.



CM 2
 CHN 76-05-1
 CHF C2 H F3 O2

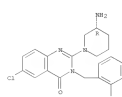


RI 940907-95-9 CAPLOS
 RI Benzonitrile, 2-[[12-[(3R)-3-amino-1-piperidinyl]-6-chloro-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1
 CHN 769157-63-3
 CHF C21 H20 Cl N5 O

Absolute stereochemistry.

L4 ANSWER 2 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)



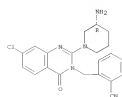
CM 2
 CHN 76-05-1
 CHF C2 H F3 O2



RI 940907-97-1 CAPLOS
 RI Benzonitrile, 2-[[12-[(3R)-3-amino-1-piperidinyl]-7-chloro-4-oxo-3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1
 CHN 940907-96-0
 CHF C21 H20 Cl N5 O

Absolute stereochemistry.



CM 2

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

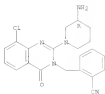
CHN 76-05-1
CHF C2 H F3 O2



HN 940907-99-3 CAPLUS
CN Benzonitrile, 2-[[2-[(1R)-3-amino-1-piperidinyl]-8-chloro-4-oxo-3(4R)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CHN 3
CHN 940907-98-2
CHF C21 H26 Cl N5 O

Absolute stereochemistry.

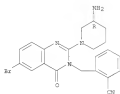


CHN 2
CHN 76-05-1
CHF C2 H F3 O2



HN 940908-00-9 CAPLUS
CN Benzonitrile,
2-[[2-[(1R)-3-amino-1-piperidinyl]-6,8-dichloro-4-oxo-3(4R)-

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



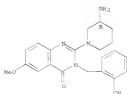
CHN 2
CHN 76-05-1
CHF C2 H F3 O2



HN 940908-02-1 CAPLUS
CN Benzonitrile, 2-[[2-[(1R)-3-amino-1-piperidinyl]-6-methoxy-4-oxo-3(4R)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CHN 3
CHN 76317-93-9
CHF C22 H23 N5 O2

Absolute stereochemistry.



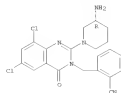
CHN 2

Hasbe

14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CHN 1
CHN 76317-92-8
CHF C21 H19 Cl2 N5 O

Absolute stereochemistry.



CHN 2
CHN 76-05-1
CHF C2 H F3 O2



HN 940908-01-0 CAPLUS
CN Benzonitrile, 2-[[2-[(1R)-3-amino-1-piperidinyl]-6-bromo-4-oxo-3(4R)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CHN 1
CHN 76317-89-3
CHF C21 H20 N5 O

Absolute stereochemistry.

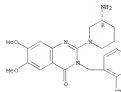
14 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

CHN 76-05-1
CHF C2 H F3 O2



HN 940908-03-2 CAPLUS
CN Benzonitrile,
2-[[2-[(1R)-3-amino-1-piperidinyl]-6,7-dimethoxy-4-oxo-3(4R)-quinazolinyl]methyl]-, (CA INDEX NAME)

Absolute stereochemistry.



HN 940908-05-4 CAPLUS
CN Benzonitrile, 2-[[2-[(1R)-3-amino-1-piperidinyl]-8-methoxy-4-oxo-3(4R)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CHN 1
CHN 940908-04-3
CHF C21 H23 N5 O2

Absolute stereochemistry.

(Continued)



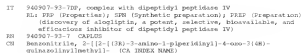
CH 1
C929 769157-95-1
C929 C25 H27 F N6 O2

Absolute stereochemistry.

(Cont. 5/19/92)

RECORD. ALL CITATIONS AVAILABLE IN THE RE

(Continued)



Absolute stereochemistry.



ACCESSION NUMBER: 2004:057326 CAPLUS

TITLE: Dipeptidyl peptidase inhibitors
INVENTOR(S): Feng, Jun; Gwaltney, Stephen L.; Kaldor, Stephen W.;
Stafford, Jeffrey A.; Wallace, Michael B.; Zhang,
Zhiyuan

PATENT ASSIGNEE(S): Syrex, Inc., USA
SOURCE: PCT Int. Appl., 244 pp
CODING: PIXX02
DOCUMENT TYPE: Patent

FAMILY SOC. SERV. CO.

| PATENT NO. | KIND DATE | APPLICATION NO. | DATE |
|---|--|--|--|
| NO 00040087053 | A1 | 200410124 | 20204324 |
| NO 00040087054 | US | 0041111 | 20204324 |
| NO 00040087055 | A1 | 200808251 | 20204324 |
| MI AB, AG, AL, AN, AT, AU, BE, BG, BR, CA, CH, CN, CO, CR, CU, CY, DE, DK, EA, EP, ES, FI, FR, GB, GR, GU, HK, IL, IN, JP, KR, LI, LU, MC, MG, MK, NL, NO, NZ, OM, PG, PL, PT, RU, SE, SG, SI, SK, ST, SW, TH, TR, UA, US, VN, YU, ZA | AB, AG, AL, AN, AT, AU, BE, BG, BR, CA, CH, CN, CO, CR, CU, CY, DE, DK, EA, EP, ES, FI, FR, GB, GR, GU, HK, IL, IN, JP, KR, LI, LU, MC, MG, MK, NL, NO, NZ, OM, PG, PL, PT, RU, SE, SG, SI, SK, ST, SW, TH, TR, UA, US, VN, YU, ZA | AB, BR, BG, BR, BW, BY, CA, CH, CN, CO, CR, CU, CY, DE, DK, EA, EP, ES, FI, FR, GB, GR, GU, HK, IL, IN, JP, KR, LI, LU, MC, MG, MK, NL, NO, NZ, OM, PG, PL, PT, RU, SE, SG, SI, SK, ST, SW, TH, TR, UA, US, VN, YU, ZA | CA, CH, CN, CO, CR, CU, CY, DE, DK, EA, EP, ES, FI, FR, GB, GR, GU, HK, IL, IN, JP, KR, LI, LU, MC, MG, MK, NL, NO, NZ, OM, PG, PL, PT, RU, SE, SG, SI, SK, ST, SW, TH, TR, UA, US, VN, YU, ZA |
| NO 00040087056 | A1 | 200410124 | 20204324 |
| NO 00040087057 | A1 | 200410124 | 20204324 |
| NO 00040087058 | A1 | 200410124 | 20204324 |
| NO 00040087059 | A1 | 200410124 | 20204324 |
| NO 00040087060 | A1 | 200410124 | 20204324 |
| NO 00040087061 | A1 | 200410124 | 20204324 |
| NO 00040087062 | A1 | 200410124 | 20204324 |
| NO 00040087063 | A1 | 200410124 | 20204324 |
| NO 00040087064 | A1 | 200410124 | 20204324 |
| NO 00040087065 | A1 | 200410124 | 20204324 |
| NO 00040087066 | A1 | 200410124 | 20204324 |
| NO 00040087067 | A1 | 200410124 | 20204324 |
| NO 00040087068 | A1 | 200410124 | 20204324 |
| NO 00040087069 | A1 | 200410124 | 20204324 |
| NO 00040087070 | A1 | 200410124 | 20204324 |
| NO 00040087071 | A1 | 200410124 | 20204324 |
| NO 00040087072 | A1 | 200410124 | 20204324 |
| NO 00040087073 | A1 | 200410124 | 20204324 |
| NO 00040087074 | A1 | 200410124 | 20204324 |
| NO 00040087075 | A1 | 200410124 | 20204324 |
| NO 00040087076 | A1 | 200410124 | 20204324 |
| NO 00040087077 | A1 | 200410124 | 20204324 |
| NO 00040087078 | A1 | 200410124 | 20204324 |
| NO 00040087079 | A1 | 200410124 | 20204324 |
| NO 00040087080 | A1 | 200410124 | 20204324 |
| NO 00040087081 | A1 | 200410124 | 20204324 |
| NO 00040087082 | A1 | 200410124 | 20204324 |
| NO 00040087083 | A1 | 200410124 | 20204324 |
| NO 00040087084 | A1 | 200410124 | 20204324 |
| NO 00040087085 | A1 | 200410124 | 20204324 |
| NO 00040087086 | A1 | 200410124 | 20204324 |
| NO 00040087087 | A1 | 200410124 | 20204324 |
| NO 00040087088 | A1 | 200410124 | 20204324 |
| NO 00040087089 | A1 | 200410124 | 20204324 |
| NO 00040087090 | A1 | 200410124 | 20204324 |
| NO 00040087091 | A1 | 200410124 | 20204324 |
| NO 00040087092 | A1 | 200410124 | 20204324 |
| NO 00040087093 | A1 | 200410124 | 20204324 |
| NO 00040087094 | A1 | 200410124 | 20204324 |
| NO 00040087095 | A1 | 200410124 | 20204324 |
| NO 00040087096 | A1 | 200410124 | 20204324 |
| NO 00040087097 | A1 | 200410124 | 20204324 |
| NO 00040087098 | A1 | 200410124 | 20204324 |
| NO 00040087099 | A1 | 200410124 | 20204324 |
| NO 00040087100 | A1 | 200410124 | 20204324 |
| NO 00040087101 | A1 | 200410124 | 20204324 |
| NO 00040087102 | A1 | 200410124 | 20204324 |
| NO 00040087103 | A1 | 200410124 | 20204324 |
| NO 00040087104 | A1 | 200410124 | 20204324 |
| NO 00040087105 | A1 | 200410124 | 20204324 |
| NO 00040087106 | A1 | 200410124 | 20204324 |
| NO 00040087107 | A1 | 200410124 | 20204324 |
| NO 00040087108 | A1 | 200410124 | 20204324 |
| NO 00040087109 | A1 | 200410124 | 20204324 |
| NO 00040087110 | A1 | 200410124 | 20204324 |
| NO 00040087111 | A1 | 200410124 | 20204324 |
| NO 00040087112 | A1 | 200410124 | 20204324 |
| NO 00040087113 | A1 | 200410124 | 20204324 |
| NO 00040087114 | A1 | 200410124 | 20204324 |
| NO 00040087115 | A1 | 200410124 | 20204324 |

OTHER SOURCE(S): MARPAT 141-309639
GZ

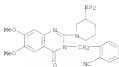


14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)
[substituted]-3-7-membered ring; R₃,R₄ = taken together form a [substituted]-5-6-membered ring; R₅ = H, [substituted]alkyl, cycloalkyl, etc.; R₆ = [substituted]C(2-7-ynylalkyl or aryl) as discussed. Thus, 2-[[2-(3-aminopiperidin-1-yl)-6,7-dimethoxy-4-oxo-6H-quinazolin-3-ylmethyl]benzonitrile] (1; R₁ = 3-cyanophenylmethyl; R₂ = 3-aminopiperidin-1-yl; R₃,R₄ = dimethoxyphenyl) was synthesized. This compound exhibited enhanced stability in rat liver microsomes.

70 769157-54-2P 769157-55-2P 769157-56-4P
769157-57-5P 769157-58-4P 769157-59-7P
769157-61-3P 769157-64-5P 769157-71-3P
769157-81-5P 769157-89-3P 769157-91-7P
769157-92-8P 769157-93-9P 769157-94-0P
769157-95-1P 769158-01-2P 769158-02-3P
769158-03-4P 769158-04-5P 769158-05-6P
769158-06-7P 769158-14-7P
3a. NME (Biological study), UCLAS (Synthetic preparation),
BIOA (Biological study), PKPP (Preparation)
(diagram) anti-depressant inhibitors
70 769157-54-2 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-4-oxo-3(4H)-
quinazolinyl]methyl]- (CA INDEX NAME)

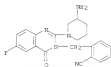


70 769157-55-3 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-6,7-dimethoxy-4-oxo-3(4H)-
quinazolinyl]methyl]- (CA INDEX NAME)



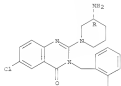
70 769157-56-4 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-8-methoxy-4-oxo-3(4H)-
quinazolinyl]methyl]- (CA INDEX NAME)

14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)



70 769157-63-3 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-6-chloro-4-oxo-3(4H)-
quinazolinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



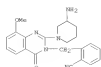
70 769157-63-3 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-7-fluoro-6-methoxy-4-oxo-
3(4H)-quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX
NAME)

CH 1

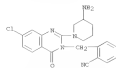
CN 769157-64-4
CMF C22 R22 F R3 O2

Absolute stereochemistry.

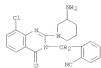
14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)



70 769157-57-5 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-7-chloro-4-oxo-3(4H)-
quinazolinyl]methyl]- (CA INDEX NAME)

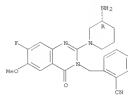


70 769157-58-6 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-8-chloro-4-oxo-3(4H)-
quinazolinyl]methyl]- (CA INDEX NAME)



70 769157-59-7 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-6-fluoro-4-oxo-3(4H)-
quinazolinyl]methyl]- (CA INDEX NAME)

14 ANSWER 3 OF 4 CAPLOS COPYRIGHT 2009 ACS on STN (Continued)



CH 2

CN 76-05-1
CMF C2 H F3 O2

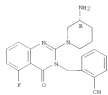


70 769157-71-3 CAPLOS
CN Benzonitrile, 2-[[2-(3-amino-1-piperidinyl)-5-fluoro-4-oxo-3(4H)-
quinazolinyl]methyl]-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CH 1

CN 769157-70-2
CMF C12 R20 F R3 O

Absolute stereochemistry.

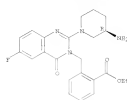


CH 2

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

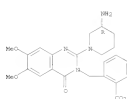
RD 769159-03-4 CAPLUS
 CD Benzoic acid, 2-[[2-[(3R)-3-amino-1-piperidinyl]-6-fluoro-4-oxo-3(4H)-quinazolinyl]methyl]-, ethyl ester (CA INDEX NAME)

Absolute stereochemistry.



RD 769159-04-5 CAPLUS
 CD Benzoic acid, 2-[[2-[(3R)-3-amino-1-piperidinyl]-6,7-dimethoxy-4-oxo-3(4H)-quinazolinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



RD 769159-05-6 CAPLUS
 CD Benzoic acid, 2-[[2-[(3R)-3-amino-1-piperidinyl]-6-fluoro-4-oxo-3(4H)-quinazolinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2021143405 CAPLUS
 DOCUMENT NUMBER: 139106649
 TITLE: Solid-phase synthesis of quinazolin-4(3H)-ones with three-point diversity
 AUTHOR(S): Resarwani, A. P.; Silvestre, G. X.; Hartog, S. X.; Pandey, S.
 CORPORATE SOURCE: Medicinal Chemistry Division, Central Drug Research Institute, Lucknow, 226 001, India
 SOURCE: Tetrahedron Letters 12022, 63(32), 5579-5581
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139106649
 GI



AB A versatile method for the solid-phase synthesis of differentially substituted quinazolin-4(3H)-ones 2 (R1 = H, Ph, PhCH2; R2 = Bu, R3 = Me;

R4 = H, CH(CH3)CH3) was developed using immobilized arylguanidines. The latter were obtained by treating the amino group of polymer-linked aminoaryl acids with isothiocyanates R4R5 followed by coupling of resulting thiocreas with secondary amines R3R6R7. Under mild acidic conditions, these immobilized arylguanidines underwent cyclization/polymer

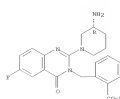
matrix cleavage to give 2 in high yields and purities.

IT 485402-04-39

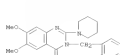
SL SP2 (Synthetic preparation) SP2P (Preparation)
 Solid-phase synthesis of (anti)quinazolinones with three points of diversity from aminoaryl carboxylic acids, isothiocyanates, and secondary amines.

RD 485402-04-8 CAPLUS
 CD 4-(3H)-Quinazolinone, 3-[(phenylmethyl)-2-[(4-[(phenylmethyl)-1-piperidinyl]- (CA INDEX NAME)

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)

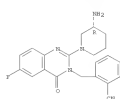


RD 769159-06-7 CAPLUS
 CD Benzonitrile, 2-[[2-[(3R)-3-amino-1-piperidinyl]-6-fluoro-4-oxo-3(4H)-quinazolinyl]methyl]- (CA INDEX NAME)

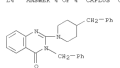


RD 769159-14-7 CAPLUS
 CD Benzonitrile, 2-[[2-[(3R)-3-amino-1-piperidinyl]-6-fluoro-4-oxo-3(4H)-quinazolinyl]methyl]- (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT